

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.89e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.85e-01

Confidence level: 7.88e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Daminozide</div> <div>Measured: 2.90e-06</div> <div>Predicted: 2.23e-05</div>	<div>Image not found</div> <div>2,4-Dichlorobiphenyl</div> <div>Measured: 2.00e-06</div> <div>Predicted: 1.51e-03</div>	<div>Image not found</div> <div>Triacontane</div> <div>Measured: 2.40e-06</div> <div>Predicted: 8.27e-11</div>
<div>Image not found</div> <div>1,1'-Biphenyl, 4,4'-dinitro-</div> <div>Measured: 2.30e-06</div> <div>Predicted: 8.64e-08</div>	<div>Image not found</div> <div>Iprobenfos</div> <div>Measured: 7.30e-06</div> <div>Predicted: 1.52e-05</div>	